μ_{eff} = effective dynamic liquid phase viscosity, Pa·s
ρ_L = liquid phase density, kg/m^3
σ = surface tension, N/m
Γ = shear stress, Pa

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Multivariable Computer Control of a Butane Hydrogenolysis Reactor

Part II: Design and On-Line Implementation of a Stochastic Controller Using an Identified Multivariate Noise Model

A multivariable stochastic controller is implemented on a pilot scale, plug flow, butane hydrogenolysis reactor. In the synthesis of the controller, a multivariate time series model of the process disturbances is used. The success of this controller is compared to a previous controller where the process disturbances are not directly modeled.

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SCOPE

Multivariable computer control of a packed-bed pilot-plant reactor has been studied by Jutan et al. (1977). A stochastic state space control algorithm was developed and implemented on the reactor in those studies. Although the multivariate stochastic disturbances entering the process were identified, they were not used in the synthesis of an optimal controller designed to specifically compensate for these disturbances. Instead, the

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disturbances were characterized arbitrarily as white noise.

In this paper, a model for the identified multivariate noise is combined with the state space dynamic model of the reactor. An optimal stochastic controller is then synthesized and implemented on the pilot reactor. The results are compared to the previous control study and some recommendations on the implications of various dynamic-stochastic modeling structures are put forward.

CONCLUSIONS AND SIGNIFICANCE

This paper has examined and compared the optimal stochastic control of a catalytic hydrogenolysis reactor using a state space model developed from mass and energy balances on the system, combined with two different assumed model structures for the stochastic disturbances that were observed in the pilot plant. In the first structure, arbitrary white noise was added to the process state equations and known measurement noise was used for the measurement equation. In the second structure, an identified disturbance was associated with process noise and measurement noise was considered negligible.

Using these two structures for noise and the model for the reactor itself, control algorithms were derived for the system. Both controllers were shown to perform well on the pilot-plant reactor. However, the first disturbance structure which better accounted for the large measurement errors that existed in temperature was seen to perform better.

Finally, a better approach was suggested which combines the two approaches by making use of the previously determined measurement noise and separately identifying the process state noise.

INTRODUCTION

Recently, there appears to be an increase in the study of process control applications to fixed-bed reactors (Silva et al. 1977; Wallman et al., 1977; Sorenson, 1977; Harris et al., 1978; Khanna and Seinfeld 1982).

Modern process control theory usually relies on obtaining a suitable process model expressed in linearized state space notation. Fixed-bed reactors are often adequately modeled only by partial differential equations and some challenge exists in obtaining a sufficiently low-order state space representation of the reactor dynamics.

In a series of papers, Jutan et al. (1977a,b,c) discussed a methodology for obtaining a state space model for a fixed-bed reactor, estimating both the dynamic and stochastic parameters from data, and finally on-line implementation of multivariate stochastic control using these models. To successfully develop a stochastic control algorithm, the stochastic nature of the process disturbances must be characterized. The control strategy, then, is designed to compensate specifically for these disturbances. In a previous paper, Jutan et al. (1977c) characterized the process disturbances by somewhat arbitrarily adding uncorrelated white noise vectors to the state space process model. The variance-covariance matrices of these white noise vectors were diagonal in structure, and two variance parameters were estimated from data and used to specify these matrices. The resulting optimal stochastic control algorithms obtained were implemented on a catalytic fixed-bed reactor. In spite of significant changes in catalyst activity, the controller performed well and had desirable robust properties.

A more direct method of characterizing the stochastic process disturbances is to model them using multivariable time-series (MacGregor and Wong, 1980). Often, the true dimensionality of the disturbance (noise) model is not equal to the dimensionality of the state space model and by use of canonical analysis (Jutan et al., 1977b), the dimensionality of the noise model can be reduced. Such a reduced noise model was developed (Jutan et al., 1977b), and the focus of the present paper is to show how this noise model was integrated into the dynamic state space reactor model using additional states to augment the original state space equation. This augmented state space equation is used to obtain an optimal stochastic control algorithm. The algorithm is implemented on the reactor and its performance is compared to that of the previous control algorithm.

REACTOR MODEL

In Part I of this series of papers (Jutan et al., 1977a), a description of the hydrogenolysis of butane over nickel on silica gel catalyst was given. For reference, the dynamic partial differential equations describing that system are repeated here.

Mass balances:

$$\frac{-G_o \partial C^i}{\epsilon L \partial z} + \frac{D_{er}}{\epsilon R^2 r} \frac{\partial}{\partial r} \frac{(r \partial C^i)}{\partial r} \frac{-\rho_B R^i}{\epsilon} = \frac{\partial C^i}{\partial t} \tag{1}$$

where $i = 1, 2, 3$ is the component number.

Energy balance: solid/gas

$$\frac{-G_o C_{pg} \rho_g}{LC} \frac{\partial T}{\partial z} + \frac{\lambda_{er}}{R^2 C r} \frac{\partial}{\partial r} \frac{(r \partial T)}{\partial r} + \frac{\sum_{i=1}^{3} \Delta h_i R_i \rho_B}{C} = \frac{\partial T}{\partial t} \tag{2}$$

where

$$C = [C_{ps} \rho_B + C_{pg} \rho_g \epsilon]$$

The system consists of three independent reactions producing propane, ethane and methane from a butane and excess hydrogen feed. A low-order linearized state space model of the dominant temperature dynamics of the system was derived as

$$\frac{d\mathbf{T}_o}{dt} = \mathbf{F}\mathbf{T}_o + \mathbf{G}\mathbf{u}$$

Discretizing this equation for a 1-min sampling interval yielded the state equations

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \tag{3}$$

where $x(t)$ is the (7×1) vector of center-line temperature deviations (T_o) at the sampling instant t.

As a result of an assumption of quasisteady state on the concentration dynamics (1), an algebraic prediction equation for concentration in terms of these temperature states (x) and the controlled flow rate (u) was obtained as

$$\mathbf{C}(t) = \mathbf{Z}\mathbf{x}(t) + \mathbf{E}\mathbf{u}(t-1) \tag{4}$$

where $C(t)$ is a (3×1) vector of radially averaged reactor effluent species compositions (deviations). Complete state temperature measurements were available from thermocouples placed along the central axis of the reactor bed, and hence the measurement equation was

$$\mathbf{y}(t) = \mathbf{I}\mathbf{x}(t)$$

Harris et al. (1980) have shown that, in practice, only one or two optimally-placed thermocouple measurements would enable equivalent state estimation and control to be achieved.

The control problem here is to design an optimal regulator for these averaged exit concentrations in the face of stochastic disturbances upsetting the system. A model for the stochastic distur-

bances must, therefore, be identified using data collected on the reactor. Since only input-output data are available, there will always be some ambiguity about the structure of any stochastic disturbance model for the states. The assumptions that one makes for the structure will have some effect on the performance of the resulting stochastic control algorithm for the unmeasured concentrations. Consider a number of possible alternative representations for the stochastic disturbances.

(i) Additive white noise vectors on the measurement and state equations.

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{w}(t) \tag{5}$$

$$\mathbf{y}(t) = \mathbf{I}\mathbf{x}(t) + \mathbf{v}(t) \tag{6}$$

Here, $w(t)$ and $v(t)$ are uncorrelated white noise vectors representing process and measurement noise respectively. This common representation for the stochastic disturbances was used in the previous control studies on the reactor Jutan et al. (1977a). There, using reactor temperature data, the covariance matrix of the measurement error was estimated as $\boldsymbol{R}_v = 4.0\,\boldsymbol{I}$ and then a single parameter β in the process noise covariance matrix $\boldsymbol{R}_w = \beta \boldsymbol{I}$ was estimated by minimizing the sum of squares of the innovations sequences. Later studies (Harris et al., 1980) using a more complex structure for $\boldsymbol{R}_w$ showed that the above uncorrelated equal variance structure for $\boldsymbol{R}_w$ was a reasonably good structure.

(ii) Colored autoregressive integrated moving average (ARIMA) noise vector on the measurement equation.

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \tag{7}$$

$$\mathbf{y}(t) = \mathbf{I}\mathbf{x}(t) + \mathbf{N}_1(t) \tag{8}$$

Here, $\boldsymbol{N}_1(t)$ represents the total effect of the stochastic disturbances occurring in the system as they appear in the measured output. An ARIMA model for $\boldsymbol{N}_1(t)$ is given by

$$\Phi(B)\mathbf{N}_1(t) = \theta(B)\mathbf{a}(t) \tag{9}$$

(where $\boldsymbol{B}\boldsymbol{N}_1(t) = \boldsymbol{N}_1(t-1)$ or an equivalent state space model

$$\mathbf{z}(t+1) = \mathbf{C}\mathbf{z}(t) + \mathbf{D}\mathbf{a}(t) \tag{10}$$

$$\mathbf{N}_1(t) = \mathbf{H}\mathbf{z}(t) \tag{11}$$

can be identified from data collected on the reactor temperatures. Nevertheless, any optimal state control scheme would be open loop since we assume that the model (and hence the states) are known exactly. Optimal output control would be more realistic with this formulation. (See discussion following (iii).) It is worth noting that stochastic disturbances are commonly identified in this form, that is, by using the residuals $\boldsymbol{N}_1(t)$ obtained by subtracting the predicted measurements $\boldsymbol{I}\boldsymbol{x}(t)$, from the experimental measurements $\boldsymbol{y}(t)$.

(iii) Colored (ARIMA) noise vector on the state equation

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{N}_2(t) \tag{12}$$

$$\mathbf{y}(t) = \mathbf{I}\mathbf{x}(t) \tag{13}$$

Here, $\boldsymbol{N}_2(t)$ can be modelled in a manner similar to case (ii) above but has been assumed to enter as real process noise in the state equation. Note that here the measurements are assumed to be error free and all the noise is considered to be true process noise.

(iv) White measurement noise and colored process noise

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{N}_3(t) \tag{14}$$

$$\mathbf{y}(t) = \mathbf{I}\mathbf{x}(t) + \mathbf{v}(t) \tag{15}$$

Once the covariance matrix $\boldsymbol{R}_v$ of the measurement noise is estimated independently from replicate measurement data, an ARIMA or state model for the process noise $\boldsymbol{N}_3(t)$ can be identified from dynamic reactor data.

Note that any of these representations can be identified from reactor data and, providing they all yield reasonably adequate predictions for the output $y(t)$, then one would obtain essentially identical output control, that is,

$$\underset{u}{\text{Min}}\, E\left\{\sum_{t=0}^{N-1} (\mathbf{y}(t)^T\mathbf{Q}\mathbf{y}(t) + \mathbf{u}(t)^T\mathbf{Q}_2\mathbf{u}(t))\right\} \tag{16}$$

from each of them. However, in terms of state control, that is,

$$\underset{u}{\text{Min}}\, E\left\{\sum_{t=0}^{N-1} (\mathbf{x}^T(t)\mathbf{Q}_1\mathbf{x}(t) + \mathbf{u}^T(t)\mathbf{Q}_2\mathbf{u}(t))\right\} \tag{17}$$

or more importantly here, concentration control (Eq. 4), the optimal controller obtained would depend on the assumed structure. As has already been pointed out, the additive white noise structure (i) was used in previous studies Jutan et al. (1977c) and achieved excellent control over the exit concentrations. This structure was physically reasonable in that a large white measurement noise $v(t)$ was shown to be present ($\boldsymbol{R}_v = 4.0\,\boldsymbol{I}$). However, the assumption of white process noise $w(t)$ might not be as reasonable.

In this paper, we use an alternative representation of the noise structure obtained in Jutan et al. (1977b) by identifying an ARIMA model for the disturbances, $N(t)$, observed in the process output. By using a canonical analysis procedure, the model for $N(t)$ is transformed into a subspace with significant colored noise and another subspace comprising white noise only. The resulting state model (in a form equivalent to that of case (iii)) is used in this paper to design and implement an optimal stochastic controller. The results are then compared with that designed and implemented using the previous additive white noise model (case (i)).

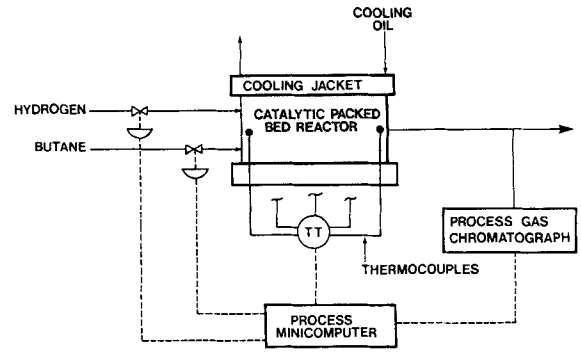

Figure 1 Reactor control configuration.

Direct Digital Control (DDC) Configuration

A description of the experimental setup as well as the process control configuration has been given by Jutan et al. (1977a). Concentration measurements from the process gas chromatograph were used to develop the model but subsequently were not implemented online as part of the control algorithms, because they were available so infrequently. Rather, the inferential equation (Eq. 4) for the average exit concentrations was used to express the objective function in terms of concentration.

In the control configuration, Figure 1, the hydrogen and butane flow rates were under DDC. These loops were sampled once per second by the system, and well-tuned digital proportional-integral (PI) control algorithms were implemented once per second by the software. The setpoints to these PI controllers were then adjusted by the multivariate algorithms every 60 seconds.

The cooling oil temperature was controlled independently by the computer. For this small reactor system, the dynamics of the coolant system were too slow to allow effective use of wall temperature as a manipulated variable. However, it was used to adjust the steady-state operating conditions in the reactor and also as a load disturbance.

Real time control software was developed using a Data General Nova 2/10 minicomputer operating under a real-time disk-operating system (RDOS).

CONTROL SYNTHESIS USING AN IDENTIFIED NOISE MODEL

In a previous paper (Jutan et al., 1977b), a multivariate time series model was obtained for the process disturbances. The dynamic stochastic state space equation was written as

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) \tag{18}$$

$$\mathbf{y}(t) = \mathbf{H}\mathbf{x}(t) + \mathbf{N}(t) \tag{19}$$

Equations 18 and 19 represent the 7th-order state space model developed in Jutan et al. (1977b), and $N(t)$ represents stochastic disturbances in the axial temperatures (x) along the reactor bed. In this form, the $N(t)$ are the residuals or differences between the observed outputs and the deterministic model and can be conveniently identified as a time series model from the sequence of residuals. Also, the predictive relationship between the exit concentrations C and the states x and flow rates u was developed (Eq. 4).

$$\mathbf{C}(t) = \mathbf{Z}\mathbf{x}(t) + \mathbf{E}\mathbf{u}(t-1) \tag{20}$$

A noise model which adequately described the series $N(t)$ was a first-order autoregressive (AR) model of the form

$$\mathbf{N}(t) = \mathbf{\Phi}\mathbf{N}(t-1) + \mathbf{a}(t) \tag{21}$$

This model was identified directly from dynamic data collected from the reactor. $a(t)$ is a white noise vector, and its covariance matrix $\mathbf{\Sigma}$ and the parameter matrix $\mathbf{\Phi}$ of the autoregressive model were estimated using linear regression Jutan et al. (1977b).

Using a canonical analysis procedure on this time series model, a set of eigenvectors (contained in a matrix L) were obtained by Jutan et al. (1977b) which reduced the dimension of the $N(t)$ vector to three. Given the 7-dimensional noise series using the L matrix of eigenvectors, two sets of series $N_A(t)$ and $N_B(t)$ were obtained, where $N_A(t)$ is a 3-dimensional noise vector with AR(1) structure and $N_B(t)$ is a 4-dimensional white noise vector containing no significant forecastable information; we have from Eq. 21

$$\begin{aligned}\dot{\mathbf{N}}(t) &= \mathbf{L}\mathbf{N}(t) = (\mathbf{L}\mathbf{\Phi}\mathbf{L}^{-1})\mathbf{L}\mathbf{N}(t-1) + \mathbf{L}\mathbf{a}(t) \\ &= \dot{\mathbf{\Phi}}\dot{\mathbf{N}}(t-1) + \dot{\mathbf{a}}(t)\end{aligned} \tag{22}$$

$$\dot{\mathbf{N}}(t) = \begin{bmatrix} \dot{N}_A(t) \\ \dot{N}_B(t) \end{bmatrix} = \begin{bmatrix} N_1(t) \\ N_2(t) \\ N_3(t) \\ N_4(t) \\ N_5(t) \\ N_6(t) \\ N_7(t) \end{bmatrix} = \begin{bmatrix} \dot{\Phi}_3 & \mathbf{O} \\ \mathbf{O} & \mathbf{O}_4 \end{bmatrix} \dot{\mathbf{N}}(t-1) + \begin{bmatrix} \dot{a}_A(t) \\ \dot{a}_B(t) \end{bmatrix} \begin{matrix} 3 \\ 4 \end{matrix} \tag{23}$$

Augmented State Equation

The reduction of the noise model from seven dimensions to three implies that we need only measure three linear combinations of the original seven temperatures to obtain all the significant information to reconstruct the noise model. The three linear combinations (Jutan et al., 1977b) are given by the first 3 eigenvectors in matrix L.

We can use L then to rewrite the state equation (Eqs. 19, 21) in terms of the new canonical variates defined as

$$\begin{aligned}\dot{\mathbf{y}} &= \mathbf{L}\mathbf{y} \\ \dot{\mathbf{N}} &= \mathbf{L}\mathbf{N}\end{aligned} \tag{24}$$

multiplying Eq. 19 by L (7×7) and making use of Eq. 23 we get

$$\mathbf{L}\mathbf{y}(t) = \dot{\mathbf{y}} = \mathbf{L}\mathbf{H}\mathbf{x}(t) + \mathbf{L}\mathbf{N}(t)$$

$$\dot{\mathbf{y}}(t) = \dot{\mathbf{H}}\mathbf{x}(t) + \begin{bmatrix} \dot{N}_A(t) \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ \dot{a}_B(t) \end{bmatrix}$$

Defining

$$\mathbf{x}^* = \begin{bmatrix} \mathbf{x}(t) \\ \dot{N}_A(t) \end{bmatrix} \begin{matrix} 7 \\ 3 \end{matrix} \qquad \mathbf{H}^* = 7\begin{bmatrix} \overset{7}{\dot{\mathbf{H}}} & \overset{3}{\mathbf{I}_3} \\ & 0 \end{bmatrix}$$

and $\mathbf{v}^*(t) = \begin{bmatrix} 0 \\ \dot{a}_B(t) \end{bmatrix} \begin{matrix} 3 \\ 4 \end{matrix}$

We can write the state space measurement equation (Eq. 6) as

$$\dot{\mathbf{y}}^{(t)} = \mathbf{H}^*\mathbf{x}^*(t) + \mathbf{v}^*(t) \tag{25}$$

For the model equation (Eq. 5), we define

$$\mathbf{A}^* = 7\begin{bmatrix} \overset{7}{\mathbf{A}} & \overset{3}{\mathbf{O}} \\ 3\begin{bmatrix} \mathbf{O} & \mathbf{\Phi}_3 \end{bmatrix} \end{bmatrix} \qquad \mathbf{B}^* = \begin{bmatrix} \mathbf{B} \\ \mathbf{O} \end{bmatrix} \begin{matrix} 7 \\ 3 \end{matrix}$$

and $\mathbf{w}^* = \begin{bmatrix} \mathbf{O} \\ \dot{\mathbf{a}}_A(t) \end{bmatrix} \begin{matrix} 7 \\ 3 \end{matrix}$

We obtain the augmented state equation (10×10) as

$$\mathbf{x}^*(t+1) = \mathbf{A}^*\mathbf{x}^*(t) + \mathbf{B}^*\mathbf{u}(t-1) + \mathbf{w}^*(t) \tag{26}$$

The dimension of the augmented state equation is equal to dimensions of the original state equation plus the dimension of the noise model. Without the use of canonical analysis, the augmented state model would have been 14th order.

The variance-covariance matrices of the model noise $w^*(t)$ and measurement noise are obtained from Eq. 7 as

$$\mathbf{R}_{v^*} = \begin{bmatrix} \mathbf{O}_3 & \\ & \mathbf{I}_4 \end{bmatrix} \text{ and } \mathbf{R}_{w^*} = \begin{bmatrix} \mathbf{O}_7 & \\ & \mathbf{I}_3 \end{bmatrix} \tag{27}$$

The unity matrices result from the normalization of the eigenvectors in the canonical analysis (Jutan et al., 1977b). Equations 25 and 26 now represent the complete dynamic stochastic state space model where both the dynamic and stochastic parameters have been estimated from reactor data.

Objective Function

Although we measure temperatures easily and rapidly, we are, in fact, interested in controlling the exit concentrations of the reactor which determine the quality of the products and the selectivity of the reaction. The objective function is thus written as

$$\text{Min } E\left(\sum_{t=0}^{N-1} (\mathbf{C}^T(t)\mathbf{C}(t) + \mathbf{u}^T(t)\mathbf{Q}\mathbf{u}(t))\right) \tag{28}$$

Concentrations are predicted theoretically from Eq. 4 as

$$\mathbf{C} = \mathbf{Z}\mathbf{x}(t) + \mathbf{E}\mathbf{u}(t-1) \tag{4}$$

The observed concentrations, if they were available at each sampling time t, would be modelled as (using Eq. 4)

$$\mathbf{C} = \mathbf{Z}\mathbf{x}(t) + \mathbf{E}\mathbf{u}(t-1) + \mathbf{M}(t) \tag{29}$$

Where $M(t)$ is a multivariable noise model for concentration disturbances analogous to $N(t)$ for the temperatures. However, since actual concentrations are not measured we have no direct information on the stochastic disturbances in concentrations. But a disturbance model on temperatures has already been identified from the temperature measurements. If we make the assumption that all the identified temperature disturbances are real variations in the process as distinct from measurement error, by Eq. 4 these will also all be propagated into $C(t)$ according to

$$\begin{aligned}\mathbf{C}(t) &= \mathbf{Z}\mathbf{y}(t) + \mathbf{E}\mathbf{u}(t-1) \\ &= \mathbf{Z}(\mathbf{H}\mathbf{x}(t) + \mathbf{N}(t)) + \mathbf{E}\mathbf{u}(t-1) \\ &= \mathbf{Z}\mathbf{x}(t) + \mathbf{E}\mathbf{u}(t-1) + \mathbf{Z}\mathbf{N}(t)\end{aligned} \tag{30}$$

since $\mathbf{H} = \mathbf{I}$

It can easily be shown that this assumption is equivalent to having modeled the temperature state equations in the form given in case (iii) of, equations 12 and 13, where the entire colored disturbance

is modelled as entering directly into the state equation, and $C(t)$ is predicted according to Eq. 4. We can obtain C as a function of the augmented state vector x^* and L as follows:

$$\text{Let } C = Zx + Eu + ZL^{-1}LN \text{ from Eq. 30}$$

$$\begin{matrix} & 3 & & 4 \end{matrix}$$

$$\text{define } ZL^{-1} = 3[(ZL^{-1})_A : (ZL^{-1})_B]$$

$$e(t) = (ZL^{-1})_B \quad \dot{a}_B(t)$$

$$\text{then } C(t) = Z^*x^*(t) + Eu(t-1) + e(t) \tag{31}$$

$$\text{where } Z^* = [Z:(ZL^{-1})_A]$$

Optimal Stochastic Control Equations

The steady-state optimal stochastic controller which minimizes the objective function (Eq. 28) after substituting Eq. 31 for C^* is well known (Astrom, 1970) and is given by

$$u(t) = L_\infty \hat{x}^*(t|t) \tag{32}$$

where L_∞ is obtained by iterating the Riccati equation until convergence.

The state estimate $\hat{x}^*$ is obtained as the solution to the Kalman filter equations. For this 10 × 10 model, because of the simple structure of R_{v^*} and R_{w^*}, the steady-state Kalman gain, K_∞ is given by

$$K_\infty = \begin{matrix} 7 \\ 3 \end{matrix}\begin{bmatrix} O_7 \\ I_3 \quad O \end{bmatrix} \tag{33}$$

The input constraint matrix Q in Eq. 28 was identical to the one used in Jutan et al. (1977) where the seventh-order model was used to obtain a control algorithm for the reactor.

DDC Control Studies

The controller is designed to minimize the variation of the exit concentrations from their set points subject to constraints on the manipulated variables (inlet flow rates) (Eq. 28). In the previous paper (Jutan et al., 1977c), a process control run was performed using the 7th-order algorithm developed from arbitrarily adding white noise to the state space model.

The performance index

$$J = \sum_t C^T(t)C(t) \tag{34}$$

was used to compare this controller with that of a single loop PID controller. The reactions are highly exothermic and under open-loop conditions reactor runaway was commonly experienced.

The control run for the 7th-order control algorithm is given in Figure 2 for comparison with the control run using the 10th-order (Figure 3) algorithm derived here.

For both the 7th-order algorithm and the 10th-order algorithm, the reactor was controlled subject to the inherent stochastic disturbances. Both controllers perform well by holding the exit mole fractions close to their set points. The objective function J in Eq. 34 rises to about 0.1 for the 7th-order model and to about 0.2 for the 10th-order model over the same time period (30 minutes). Control action for the 7th-order model appeared to be somewhat smoother.

Although the controllers were assigned to compensate specifically for disturbances characterized by the noise model $N(t)$, one test of robustness is to deliberately add a disturbance significantly different from $N(t)$. The most severe disturbance was a step change in the wall coolant temperature. Without control, a change of a few degrees in the wall temperature commonly caused reactor runaway with 100% conversion of the reactants.

After the first 30 minutes, a 5°C step change in the wall coolant temperature was introduced. In both cases (Figures 2 and 3), the controllers responded by sharply reducing the butane flow thus cutting off the potential supply of heat (through the exothermic reaction). The flow rate of hydrogen is increased slightly which

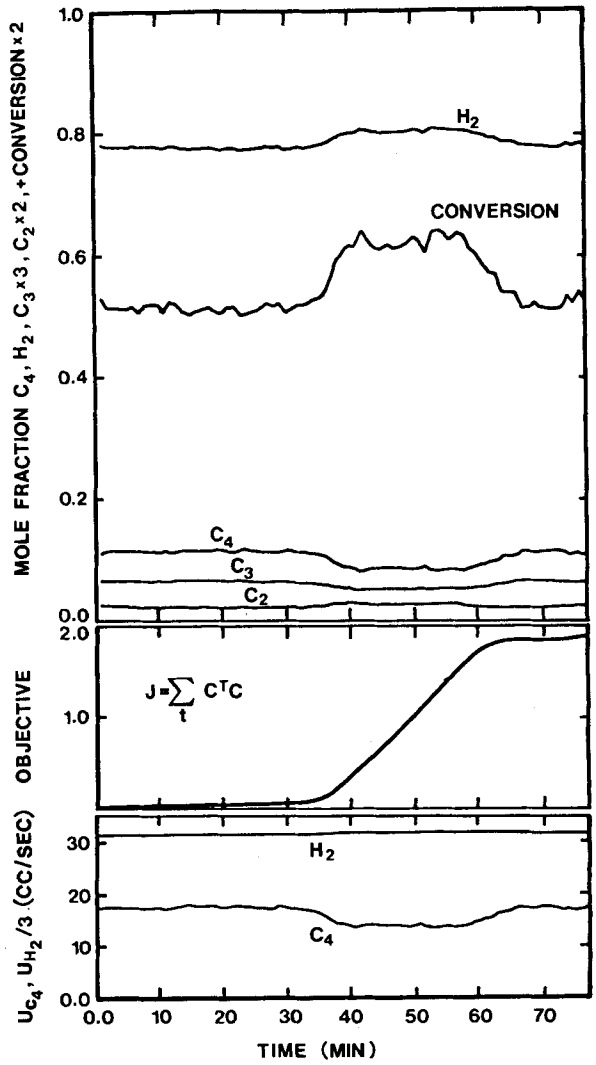

Figure 2 Control run using 7th-order algorithm.

tends to decrease the reaction rate (Jutan et al., 1977a). (Hydrogen flow scale is divided by a factor of 3 in Figures 2 and 3). The offsets for the two controllers are approximately equal as seen by comparing the conversion and mole fraction levels in Figures 2 and 3.

The objective function for the 10th-order algorithm rises to just under 3.0 for the same period (77 minutes) as the 7th-order controller where the corresponding value for the objective function is 2.0.

Comparison of the Two Controllers

The 7th-order algorithm performed better for this set of runs although both controllers were quite acceptable. A difference between the controllers has arisen because of the different manner in which the stochastic disturbances have been modeled. One would expect the control based on the most realistic disturbance model to perform better.

The 7th-order model accounted for white measurement noise but somewhat arbitrarily assumed a white process or state noise.

The 10th-order model was developed using a disturbance model identified for the temperature measurements. Substituting this into the concentration equation (30) gave us a model form equivalent to case (iii) above, which implied that measurement noise was insignificant. Since the latter was, in fact, large ($\sigma^2 = 4°C$; Jutan et al., 1977b), this appears to have degraded the control somewhat in this case. A better approach would have been to use the known

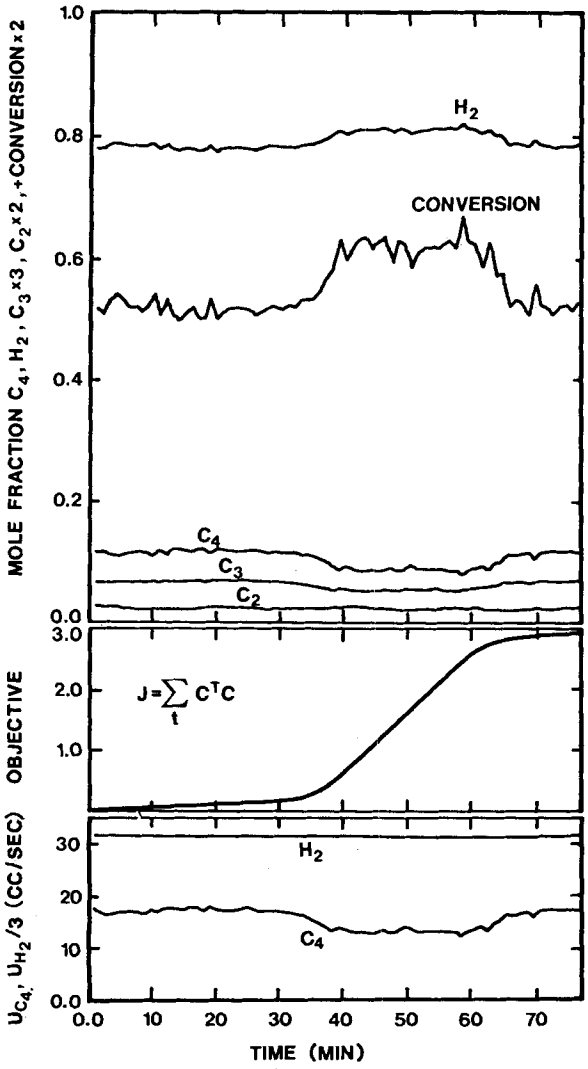

Figure 3 Control run using 10th-order algorithm.

measurement white noise and then identify a structure for the process noise as detailed in case (iv).

Another explanation for the different performance is the effect of a change in catalyst activity on the accuracy of a previously identified noise model.

When the dynamic and stochastic models were fitted, the data show the hotspot positioned towards the exit end of the reactor (83% of the distance along the reactor). At a later stage, when the control run was performed, the hotspot had moved (due to a drop in catalyst activity) towards the center of the reactor.

In deriving and fitting the canonical noise model, most of the activity was assigned to a hotspot closer to the end of the reactor (Jutan et al., 1977b). This canonical reduction would not apply precisely to the conditions under which the reactor was being controlled. This would cause some loss in the quality of control.

The 7th-order controller was derived using diagonal matrices for R_v and R_ω (the covariance matrices of the noise) with equal elements along the diagonal. This, in effect, spreads the magnitude of the disturbances equally across all the temperatures. Should the position of hotspot temperature change significantly, it would still be given equal weight in the Kalman filter.

ACKNOWLEDGMENT

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NOTATION

$\mathbf{A}$	= $n \times n$ dynamic state matrix (Eq. 5)
C^i	= concentration of species i, mol/cm^3
$\bar{C}^i$	= radial average concentration of species i, mol/cm^3
C_{ps}	= specific heat of solid, J/kg·K
C_{pg}	= specific heat of gas, J/kg·K
C	= specific heat term $[C_{ps}\rho_B + C_{pg}\rho_g\epsilon]$ (Eq. 2)
D_{er}	= effective radial diffusivity (based on empty reactor volume, m^2/s)
$E[\cdot]$	= expectation operator
G_o	= superficial gas velocity, m^3 gas (m^2 reactors)
$\boldsymbol{H}$	= $m \times n$ measurement matrix (Eq. 19)
I_m	= mth-order unity matrix
$\boldsymbol{K}_\infty$	= steady-state Kalman gain matrix (Eq. 33)
L	= reactor length, m
$\boldsymbol{L}_\infty$	= optimal steady state feedback gain matrix (Eq. 32)
$\boldsymbol{N}(t)$	= residual noise vector
$\boldsymbol{Q}$	= weighting matrices, optimal controller designs
r	= radial distance in reactor (normalized)
R^i	= net reaction rate for species i, mol/(kg catalyst·s)
$\boldsymbol{R}_w$	= variance covariance matrix for $\boldsymbol{w}(t)$ (Eq. 5)
$\boldsymbol{R}_v$	= variance covariance matrix for $\boldsymbol{v}(t)$ (Eq. 6)
T	= homogeneous gas/solid temperature, Eq. 2, K
T_o	= temperature along centre axis of reactor, K
t	= time: continuous (s); discrete (min)
$\boldsymbol{u}$	= vector of manipulated variables
$\boldsymbol{v}(t)$	= white measurement noise sequence (Eq. 6)
$\boldsymbol{w}(t)$	= white generating noise sequence (Eq. 5)
$\boldsymbol{x}(t)$	= state vector at sample time t
$\boldsymbol{x}(t\|t)$	= state estimate (simultaneous of $\boldsymbol{x}$)
$\boldsymbol{y}$	= vector of output variables
z	= axial distance along reactor (normalized)

Greek Letters

λ_{er}	= effective radial thermal conductivity, W/(m·K)
ρ_B	= bulk density of catalyst, kg/m^3
ρ_g	= gas density, kg/m^3
Δh_i	= heat of reactor for reaction i, J/mol
ϵ	= void fraction, m^3 gas in voids/m^3 empty reactor
Φ	= state transition matrix for noise model (Eq. 21)
σ	= standard deviation
τ	= time

Special Symbols

T	= transpose of matrix or vector
$\wedge$	= estimate
$\cdot$	= linear transformation (Eq. 24)

Subscripts

ex	= exit conditions for reactor
i	= species number
o	= center axial conditions
∞	= steady-state value

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Optimal Operation of Integrated Processing Systems

Part II: Closed-Loop On-Line Optimizing Control

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A method for tracking the economically optimal operating conditions of a chemical process in the presence of constraints is developed. The technique is based on an on-line search rather than a fundamental model. The most profitable operating point is found by fitting a dynamic model of the process based on data obtained from experimental moves on the plant.

This model is used to compute gradients of the economic objective and of the constraints so that a direction of economic improvement inside the allowed operating region of the plant is always obtained. Constraint violations during the transients are prevented by a multivariable regulator. A new regulation method (Internal Model Control) is used which permits explicit handling of constraints and which can be made robust against modelling errors. This combined optimization/regulation approach is tested in a demonstrative simulation example and shown to be reliable for following a moving optimum and safely handling complex constraint moves.

SCOPE

In the presence of disturbances, the optimal operating point of a process usually shifts from one set of active constraints to another. To keep the operation close to the constraints without violating them, regulatory controllers are generally employed. A standard approach for transfering the operation from one point to another is to switch between different sets of Single Input-Single Output (SISO) loops to tie the constraints which become active (Arkun, 1979). However, due to dynamic interactions and plant changes the SISO loops are difficult to tune and likely to become unstable, rendering the switching procedure unreliable.

In this paper a multivariable control scheme is suggested which considers all constraints, outputs and manipulated variables simultaneously. Since it takes into account all interactions, the transfer of operating points occurs smoothly. The scheme also allows to enhance the robustness in the face of changes in the process. This regulator interfaces with the adaptive on-line optimization algorithm introduced in Part I of this series (Garcia and Morari, 1981) to produce a method which addresses the overall control requirements of a process. A simulation example shows the ability of the scheme to safely track the optimal operating point of a plant in the event of nontrivial constraint shifts.

CONCLUSIONS AND SIGNIFICANCE

A new optimizing controller for plants with constraints was developed. A simulation example of a benzene production plant was used to demonstrate the ability of the scheme to keep the operation at its economically optimal conditions as constraints are shifted due to unmeasured disturbances. The on-line optimizer based on an identified dynamic model of the plant was shown to exhibit fast speed of tracking and to be reliable to

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